Laboratory Name: National Renewable Energy Lab
B&R Code: KC020103

FWP and possible subtask under FWP:
Novel Ordered Semiconductor Alloys

FWP Number:
ER20

Program Scope:
The research on this project involving ordered semiconductor alloys combines experimental and theoretical efforts aimed at understanding long-range order in isovalent semiconductor alloys. The project includes: (i) MOCVD growth of III-V alloys such as GaP/InP, AlP/GaP, AlP/InP, AlAs/InAs, and GaAs/GaP, (ii) Raman, modulation reflectance, photoluminescence, NSOM, Magneto-PL and reflectance-difference spectroscopy studies of ordering in the above systems, and (iii) first-principles theoretical studies of surface-induced, epitaxially-induced and bulk ordering in various alloys as well as on the electronic bandstructure changes and lattice dynamics changes induced by ordering. The project includes structural studies based on transmission electron diffraction and X-ray scattering for determining the order parameter and involves use of DOE synchrotron facilities.

Major Program Achievements (over duration of support):
Developed the concept of partial ordering, statistical distribution function and order parameter, orientational superlattices, effective mass anisotropy, pyroelectric behavior and spontaneous electric fields. Developed theoretical models for surface induced ordering. First structural and electronic measurements of order parameter. Developed ability to tailor order parameter and consequent electronic properties. Developed the understanding of the lattice dynamics and phonon spectrum of ternary alloy GaInP through control of order parameter. Developed the understanding of the influence of microstructure on the optoelectronic properties of the spontaneously ordered alloy.

Program impact:
Almost all the present understanding of the electronic properties of spontaneously ordered semiconductor alloys has been pioneered by this program. This understanding had an impact on the fabrication of very high efficiency solar cells (>30%) and other solid state optoelectronic devices.

Interactions:
University of Houston (S.C. Moss), X-ray and synchrotron studies of order parameter.
Harvard University, Ballistic Electron Microscopy Studies of ordering effects on bandstructure.
Texas A&M University (M. Weimar), UHV X-STM studies of the order parameter.
NIST-Boulder (M. Keller). E-beam lithography for submicron PL studies.
Univ. of Erlangen (G. Doehler), Polarization sensitive devices based on ordered alloys.
Univ. of Stuttgart (P. Ernst), Order-Disorder heterostructures
Sandia National Labs. (E. Jones), Magneto-PL studies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Bardeen Award (A. Zunger), BES-DMS Outstanding achievement award (A. Zunger). Cover page of MRS bulletin. Organized APS-2000 Focus Session Symposium on Ordering, Organized MRS Symposia related to Spontaneous Ordering in 1995 and 1999. Book on "Spontaneous Ordering in Semiconductor Alloys" by Plenum/Kluwer, Edited by A. Mascarenhas in 2002. Over 100 Physical Review publications and over 10 Physical Review Letters on the subject of Spontaneous Ordering, Over 15 Invited Talks.

Personnel Commitments for FY2002 to Nearest +/- 10%:
Y. Zhang (80%), W. McMahon (70%), M. Hanna (40%), 2 postdocs. (100%).

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $713K **FY01 BA $664K** **FY02 BA $651K**

Laboratory Name: National Renewable Energy Laboratory
B&R Code: KC02.0103

FWP and possible subtask under FWP:
ER0K: Overcoming doping bottlenecks

FWP Number:
ERWER0K

Program Scope:
The objective of the project is to understand the doping limits in semiconductors and to suggest ways to overcome these limits, which is essential to the design of a wide range of new semiconductor devices such as high-efficiency solar cells, blue and UV LED, detector, and laser, and next-generation integrated circuits.

Major Program Achievements (over duration of support):
Developed the theory of equilibrium doping limits. From the theory, one can predict, from the doping properties of only a few semiconductors and from the band alignments of them with the others, the doping properties of a wide range of semiconductors and alloys. Developed the non-equilibrium doping theory. A number of recent important experimental observations were explained: the lack of doping limit in boron doped silicon, the p-type conductivity of zinc oxide, the mysteriously high nitrogen solubility in gallium arsenide, the p-type transparent conducting oxides, and more. Our studies are instrumental to the development of the basic understanding of the doping bottlenecks, as well as providing the practical recipes to overcome such bottlenecks in wide-gap semiconductors. Band structure engineering by impurities represents another important achievement. The studies of the oxygen induced direct-gap, visible light-emitting silicon and of the band gap tuning by hydrogen implantation in gallium arsenide nitride have added new dimensions to our already very-exciting doping project.

Program impact:
Seven papers were published in Physical Review Letters since FY00. Nature's "Materials Update" had a feature article on Aug. 8, 02 about our proposal of direct-gap, light-emitting silicon. Overall, our studies provide insights on the microscopic origin of the doping limits in semiconductors, extend the physics of semiconductor point defects into the non-equilibrium growth regime, and suggest new ways to overcome the doping limits, as well as to modify the host material properties. The work on zinc oxide is an important step in the worldwide quest of p-type conductivity in this technologically important material.

Interactions:
C. G. Van de Walle, Polo Alto Research Center, Inc.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
DOE/BES Chunky Bullet Award, 2002
Shengbai Zhang elected a Fellow of the American Physical Society
About 12 invited talks in international conferences since 1999

Personnel Commitments for FY2002 to Nearest +/- 10%:
Shengbai Zhang (Principal Investigator) 5%
Su-Huai Wei (co-PI) 5%
Alex Zunger (co-PI) 5%
Xuan Luo (post-doc) 100%
Xilian Nie (post-doc) 100%
Cetin Kilic (post-doc) 100%

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $354,000 **FY01 BA** $329,000 **FY02 BA** $322,000

Laboratory Name: National Renewable Energy Lab
B&R Code: KC020202

FWP and possible subtask under FWP:
Physics of isoelectronic co-doping

FWP Number:
ER2B

Program Scope:
Isoelectronic co-doping GaAs and GaP with Bismuth and Nitrogen is proposed as a novel method for regularizing the abnormal alloy behavior that is observed in these materials when they are doped with Nitrogen alone. The technique will lead to enhancements in 1) the solubility of isoelectronic dopants, and 2) carrier mobilities as compared to doping with Nitrogen alone. The use of the technique will make it possible in several situations to overcome the limitations imposed by semiconductor alloy constraints on the design of some technological important devices such as such as solar cells, lasers and LED's. Most importantly, it will enable the growth of photonic devices on Silicon substrates. The proposed research will advance the basic understanding of the Mott-transition in heavily doped semiconductors as well as help unravel the fundamental mechanisms of alloy formation.

Major Program Achievements (over duration of support):
First direct observation of Nitrogen resonant level as well as simultaneously of isolated Nitrogen impurity level, of effective mass anomalies, of giant bandgap bowing in GaP, and of the impurity band model. Invention of the concept of isoelectronic co-doping for regularizing optoelectronic properties of GaAs:N and GaP:N. First successful incorporation of Bi into GaAs that showed isoelectronic trap like behavior. The technique of resonant light scattering for probing localized electronic states was pioneered under this project.

Program impact:
The research resulting from this project has set the trend for most of the current perspective of the mechanisms underlying the giant bandgap bowing in dilute Nitride Alloys. A patent with 135 claims for optoelectronic devices based on the invention of the concept of isoelectrnic co-doping has been filed.

Interactions:
Univ. of California San Diego, Growth of GaP:N and GaAs:N
Univ. of British Columbia, Growth of GaAs:Bi
Univ. of Montreal, Rutherford Backscattering studies.
Institute of Semiconductors (Chinese Acad. Of Sciences), Ultrafast studies
National High Magnetic Field Lab., Florida State Univ., High Magnetic Field Studies
Iowa State Univ., High Pressure Studies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Three Invited Talks, 4 Invited Papers, 21 research publications (1 Phys. Rev Lett.)

Personnel Commitments for FY2002 to Nearest +/- 10%:
Y. Zhang(10%), Graduate Student (50%), 1.5 Postdoc.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $ 0K **FY01 BA $ 0 K** **FY02 BA $200K**

Laboratory Name: National Renewable Energy Lab
B&R Code: KC020202

FWP and possible subtask under FWP:
Composition Modulation in Semiconductor Alloys

FWP Number:
ER60

Program Scope:
This project deals with growth, structural characterization and optical characterization of the phenomenon of spontaneous composition modulation in semiconductor alloys. The phenomenon is being investigated in AlAs/InAs short period superlattices grown by MBE as well as AlInAs epilayers grown by MOCVD. The polarization anisotropy exhibited by these materials, and the changes in the emission energies resulting from the composition amplitude swings is investigated. The ability to control the superposition of two orthogonal modulation waves is being researched with respect to applications for 2-D templates for organized quantum dot arrays.

Major Program Achievements (over duration of support):
The phenomenon of lateral composition modulation in ultra-short period semiconductor superlattices and its effects on optoelectronic properties were discovered as part of this project. The understanding of the morphological instabilities that drive the lateral composition modulation and the ability to control the process has been a major part of the achievements of this project.

Program impact:
The entire field of lateral composition modulation in short period superlattices has been pioneered through the research on this project. Several researchers worldwide have now begun working on this field, and this includes world class theorists such as P. Voorhees, J. Tersoff, and I. Ipatova. It has made it feasiblel to now design highly polarization sensitive optical devices for optical communications applications.

Interactions:
University of Houston (S.C. Moss), X-ray and synchrotron studies of Composition Modulation.
University of Oklahoma, MBE Growth of Composition Modulation semiconductor alloys.
Univ. of Erlangen (G. Doehler), Polarization sensitive devices based on Composition Modulation.
Sandia National Labs. MBE Growth, TEM and X_ray k-mapping studies of Composition Modulation.
University of Michigan, Scanning Tunneling Microscopy studies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
MRS Bulletin Article on Composition Modulation. Organized MRS Symposia related to Composition Modulation in 1995 and 1999. Over 5 Invited Talks and over 25 publications on Composition Modulation.

Personnel Commitments for FY2002 to Nearest +/- 10%:
Y. Zhang(10%), Graduate Student (50%), A. Norman (40%),

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $210K **FY01 BA $205K** **FY02 BA $208K**

Laboratory Name: National Renewable Energy Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP:
Carbon Nanotube Membranes and Adsorbents for CO_2 Removal

FWP Number: ERWER0L

Program Scope:
Understand the competitive adsorption and transport of non-polar molecules in carbon nanotube powders and membranes. Tailor carbon nanotube material properties through synthesis and post-synthesis modification to optimize adsorption selectivity for particular species from mixed gases. Design and construct membranes that offer high selectivity and throughput for separation of CO_2 and CH_4, separation of O_2 and N_2, and the purification of H_2 containing streams.

Major Program Achievements (over duration of support):
Temperature programmed desorption studies of CO_2 and CH_4 binding: Purified, laser-grown carbon single-wall nanotube (SWNT) powders strongly bind CO_2 and only weakly adsorb CH_4 at room temperature and 500 torr. D_2 was found to desorb at a temperature approximately 50 degrees higher than H_2. These adsorption studies indicate that selective transport separations will be possible in the membrane configuration.

Chemical vapor deposition (CVD) growth of SWNTs: Developed supported Fe:Mo catalyst for SWNT growth from methane/hydrogen at low-temperatures near the thermodynamic carbon deposition boundary for this system. Control of CH_4 mass transport to the catalyst surface while directing SWNT growth away permits continuous growth. Raman spectroscopy shows that ~90% of the tubes produced are of the zig-zag variety. The gas separation properties of chromatograph columns packed with CVD-grown SWNTs are currently under study.

Membranes: Carbon nanotubes have been formed into membranes as either (i) neat, purified, SWNT papers; (ii) SWNTs dispersed into a variety of polymer binders, and (iii) carbon nanotubes grown-in or supported-by anodically-grown porous alumina films. First membrane transport experiments showed deviation from Knudsen flow and evidence for molecular sieving. SWNTs in Nafion binder behave as "artificial muscle".

Program impact:
Challenge the idea that efficient gas separations must be done using small pores of molecular dimensions. Design membranes that utilize the adsorption of non-polar species on pore walls having polarizable electron densities and tunable electronic properties.

Interactions:
External: J. K. Johnson (U. of Pittsburgh) and D.S. Sholl (Carnegie Mellon) - gas transport theory in SWNTs; T. Gennett (Rochester Institute of Technology) – polymer composites; R. Hallock (U. Mass) – low temperature hydrogen adsorption; IEA Annex 17 members – hydrogen adsorption; R. Chahine (U. Quebec, Trois-Rivieres, Canada) volumetric adsorption measurements; G. Pez (Air Products) – theory and materials preparation.
Internal: Effort is synergistic with a funded DOE EERE HFCIT program on hydrogen storage. Crada with Honda R&D Americas through DOE/EERE.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
International Energy Agency Annex 17 expert on hydrogen storage (M.J. Heben). Technical Lead on new Carbon/Hydrogen Working Group (DOE/EERE/HFCIT), 11 invited talk since 2001.

Personnel Commitments for FY2002 to Nearest +/- 10%:

M.J. Heben (task leader) 10%; A.C. Dillon (research associate) 10%; G.L Hornyak (research associate) 70% - left project in July; L. Wagg (post-doc) 100% - joined project in May; K.E.H. Gilbert (student) 100%.

Authorized Budget (BA) for FY00, FY01, FY02:
FY00 BA $300,000 **FY01 BA** $271,000 **FY02 BA** $252,000